Review of: "Design and Molecular Screening of Various Compounds by Molecular Docking as BACE-1 Inhibitors"

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Potential competing interests: No potential competing interests to declare.

[Review Report for Qeios]

The manuscript entitled "Design and Molecular Screening of Various Compounds by Molecular Docking as BACE-1 Inhibitors" is very poorly written, and the ideas do not flow logically. The manuscript, in my view, is in a preliminary state and is inadequate for publication in its current form in the *Qeios.* This manuscript continues to be rather poor in scientific and English writing. It just looks like a random collection of data. I would encourage the authors to carry out a series of additional experimental work and submit it at a later, more advanced state. Some of my serious concerns are given below:

1. The introduction part of the manuscript is not appealing and must be revised. Cite the following papers for molecular docking simulation studies:

- https://doi.org/10.1016/j.molstruc.2022.134780
- https://doi.org/10.1080/07391102.2023.2293260
- https://doi.org/10.1007/s10534-022-00385-6

2. In the introduction, add recent data [According to the Dementia India report (2010)]. And cite its specified reference.

3. The manuscript needs reorganization and should be re-structured and complemented with more computational/experimental information. All the results are not properly discussed. Include more discussion of the results rather than simply tabulating the results.

4. The authors should also include the statistical analysis for the obtained results.

5. In the Results and Discussion section, the authors are encouraged to add appropriate justification and further explain the deduced results in light of the following articles. Also, cite them.

- https://doi.org/10.1016/j.bioorg.2019.103124
- https://doi.org/10.1016/j.molstruc.2021.131933

6. The data is not represented in a well-structured and presentable manner. The text of the manuscript must be properly aligned and formatted.

7. Ensure consistent style, font style, and size for all structures, figures, and tables.

8. There are too many figures and tables in the main file. It is recommended to provide the secondary data as supporting information.

9. Correct the unit of docking score; it should be kcal instead of Kcal, as the capital K is the unit of Kelvin, not kilo.

10. The conclusion section needs improvement. Rewrite it and make it meaningful.

11. Authors should avoid citing references more than once because citing the same references multiple times in the same article can make it look cluttered. Authors are also advised to focus on their write-up as there are many silly mistakes.